An alternative method for the calculation of joint probability distributions. Application to the expectation of the triplet invariant.

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1. Introduction

As explained in the master article this supplementary document is about the calculation of the expectation of the triplet invariant in $P1$ when sampling over all possible atomic distributions ρ that satisfy the constraints

$$
\begin{aligned}
&\langle E_{\mathbf{h}} E_{\mathbf{k}} E_{-\mathbf{h}-\mathbf{k}} \rangle_\rho = \\
&\quad \int \mathcal{D}\rho \int d\mathbf{x} d\mathbf{u} d\mathbf{v}\, \rho(\mathbf{x})\, \rho(\mathbf{x}+\mathbf{u})\, \rho(\mathbf{x}+\mathbf{v}) \exp\left[2\pi i \left(\mathbf{h}\cdot\mathbf{u} + \mathbf{k}\cdot\mathbf{v}\right)\right] \mathrm{Prob}(\rho) = \\
&\quad Cte \int \mathcal{D}\rho(\mathbf{x})\, \delta\left(\rho^2(\mathbf{x}) - \frac{\delta(\mathbf{0})}{\sqrt{N}} \rho(\mathbf{x})\right) \times \delta\left(\int d\mathbf{y}\, \rho(\mathbf{y})\, \rho(\mathbf{x}+\mathbf{y}) - P(\mathbf{x})\right) \times \\
&\quad \delta\left(\int d\mathbf{x}\, \rho(\mathbf{x}) - \sqrt{N}\right) \int d\mathbf{x} d\mathbf{u} d\mathbf{v}\, \rho(\mathbf{x})\, \rho(\mathbf{x}+\mathbf{u})\, \rho(\mathbf{x}+\mathbf{v}) \exp\left[2\pi i \left(\mathbf{h}\cdot\mathbf{u} + \mathbf{k}\cdot\mathbf{v}\right)\right]
\end{aligned}
$$

2. Formulas and Notation

1. $\rho(\mathbf{x})$ denotes the unknown atomic distribution and $P(\mathbf{x})$ the (known) Patterson function.

2. $Q(\mathbf{x}) = P(\mathbf{x}) - \delta(\mathbf{x})$

3. $K_{\mathbf{x},\mathbf{y}} = K(\mathbf{x}, \mathbf{y})$

4. $K^{-1}_{\mathbf{x},\mathbf{y}} = \left(K^{-1}\right)_{\mathbf{x},\mathbf{y}}$

5. $L^t\rho = \int d\mathbf{x}\, L\left(\mathbf{x}\right)\rho\left(\mathbf{x}\right)$

6. $\rho^t K\rho = \int d\mathbf{x}d\mathbf{y}\,\rho\left(\mathbf{x}\right)K_{\mathbf{x},\mathbf{y}}\rho\left(\mathbf{y}\right)$

7. $\det\left(AB\right) = \det A\det B$

8. $\det A = \exp\mathrm{Tr}\ln A$

9. $L_{\mathbf{x},\mathbf{y}} = \lambda\left(\mathbf{x}-\mathbf{y}\right)$

10. $M_{\mathbf{x},\mathbf{y}} = \mu\left(\mathbf{x}\right)\delta\left(\mathbf{x}-\mathbf{y}\right)$

11. $\int d\mathbf{x} = 1$

12.

$$\begin{aligned}
&\int\mathcal{D}\rho\,\exp\left[-\frac{1}{2}\rho^t K\rho - iL^t\rho\right]F\left[\rho\right] \\
&\quad = \int\mathcal{D}\rho\,\exp\left[-\frac{1}{2}\int d\mathbf{x}d\mathbf{y}\,\rho\left(\mathbf{x}\right)K\left(\mathbf{x},\mathbf{y}\right)\rho\left(\mathbf{y}\right) - i\int d\mathbf{x}\,L\left(\mathbf{x}\right)\rho\left(\mathbf{x}\right)\right]F\left[\rho\right] \\
&\quad = C\frac{1}{\sqrt{\det\mathcal{K}}}\exp\left[-\frac{1}{2}L^t\mathcal{K}^{-1}L\right]\times\exp\left[\frac{1}{2}\int\frac{\delta}{\delta\varphi\left(\mathbf{x}\right)}\mathcal{K}^{-1}_{\mathbf{x},\mathbf{y}}\frac{\delta}{\delta\varphi\left(\mathbf{y}\right)}\right]F\left[\varphi\right]\Big|_{\varphi=\varphi_0} \\
&\qquad\qquad\text{where } \varphi_0 = -i\mathcal{K}^{-1}L \text{ and } \mathcal{K} = \frac{1}{2}\left(K+K^t\right)
\end{aligned}$$

13.

$$\begin{aligned}
&\int\mathcal{D}\phi\,\exp\left[-\frac{1}{2}\int\phi K\phi\right]H\left[\phi\right]\Psi\left[\phi\right] \\
&\qquad = \frac{1}{\sqrt{\det\mathcal{K}}}\exp\left[\int\frac{\delta}{\delta\phi}\mathcal{K}^{-1}\frac{\delta}{\delta\varphi}\right]Z\left[\phi\right]\Delta\left[\varphi\right]\Big|_{\phi=\varphi=0} \qquad (1)
\end{aligned}$$

where

$$\begin{aligned}
\mathcal{K} &= \frac{1}{2}\left(K+K^t\right) \\
Z\left[\phi\right] &= \exp\left[\frac{1}{2}\int\frac{\delta}{\delta\phi}\mathcal{K}^{-1}\frac{\delta}{\delta\phi}\right]H\left[\phi\right] \\
\Delta\left[\varphi\right] &= \exp\left[\frac{1}{2}\frac{\delta}{\delta\varphi}\mathcal{K}^{-1}\frac{\delta}{\delta\varphi}\right]\Psi\left[\varphi\right] \qquad (2)
\end{aligned}$$

3. Calculation of a Gaussian integral

We shall now calculate a gaussian integral of the form $\int_{-\infty}^{\infty} d^n u \, \exp\left(-\frac{1}{2}u^t M u + L^t u\right)$ where u is a vector in $\mathbb{R}^n$, u^t is the transpose of the column vector u, $du = du^1 \dots du^n$, M is an invertible $n \times n$ matrix in $\mathbb{C}^n \times \mathbb{C}^n$ and L is a column vector in $\mathbb{C}^n$.

First we suppose that M is a positive matrix: $M > 0$. Then we want to do a transformation $u \to v$ to cancel the linear term in u. We shall try

$$u = M^{-\frac{1}{2}} v + A. \text{ (and remark that } M^t = M)$$

Then (remark that $(AB)^t = B^t A^t$)

$$\begin{aligned}
-\frac{1}{2}u^t M u + L^t u &= -\frac{1}{2}\left(M^{-\frac{1}{2}}v + A\right)^t M \left(M^{-\frac{1}{2}}v + A\right) + \\
&\quad L^t \left(M^{-\frac{1}{2}}v + A\right) \\
&= -\frac{1}{2}v^t v - \frac{1}{2}v^t M^{-\frac{1}{2}} M A - \frac{1}{2}A^t M M^{-\frac{1}{2}} v - \\
&\quad \frac{1}{2}A^t M A + L^t M^{-\frac{1}{2}} v + L^t A \\
&= -\frac{1}{2}v^t v - A^t M^{\frac{1}{2}} v - \frac{1}{2}A^t M A + \\
&\quad L^t M^{-\frac{1}{2}} v + L^t A \\
&= -\frac{1}{2}v^t v - \left(A^t M^{\frac{1}{2}} - L^t M^{-\frac{1}{2}}\right) v + \\
&\quad L^t A - \frac{1}{2}A^t M A.
\end{aligned}$$

Next we choose

$$A = M^{-1} L.$$

Then

$$\begin{aligned}
-\frac{1}{2}u^t M u + L^t u &= -\frac{1}{2}v^t v + L^t M^{-1} L - \\
&\quad \frac{1}{2}\left(M^{-1}L\right)^t M M^{-1} L \\
&= -\frac{1}{2}v^t v + \frac{1}{2}L^t M^{-1} L
\end{aligned}$$

Also the transformation $u \to v$ gives the jacobian

$$d^n u = \det M^{-\frac{1}{2}} d^n v = \frac{1}{\sqrt{\det M}}\, d^n v.$$

Thus

$$\begin{aligned}\int_{-\infty}^{\infty} d^n u \, \exp\left(-\frac{1}{2} u^t M u + L^t u\right) &= \frac{1}{\sqrt{\det M}} \int d^n v \, \exp\left(-\frac{1}{2} v^t v + \frac{1}{2} L^t M^{-1} L\right) \\ &= Cte \, \frac{1}{\sqrt{\det M}} \exp\left(\frac{1}{2} L^t M^{-1} L\right). \end{aligned} \tag{3}$$

Finally consider the general case: the M_{ij} are complex but M is invertible. The expression $\frac{1}{\sqrt{\det M}} \int d^n v \, \exp\left(\frac{1}{2} L^t M^{-1} L\right)$ is an analytic function of the complex variables (there is a branch cut because of $\sqrt{\det M}$!) M_{ij}. For positive M it is proportional to $\int_{-\infty}^{\infty} d^n u \, \exp\left(-\frac{1}{2} u^t M u + L^t u\right)$. Hence by analytical continuation it will still be proportional for all complex M_{ij} as long as M^{-1} and the integral exist.

So we get $\int d^n u \, \exp\left(-\frac{1}{2} u^t M u + L^t u\right) = Cte \, \frac{1}{\sqrt{\det M}} \exp\left(\frac{1}{2} L^t M^{-1} L\right)$.

4. Functional differentiation

Let $F[\rho]$ be a functional of some function ρ, e.g. $F[\rho] = \int d\mathbf{x}\, f(\mathbf{x})\, \rho(\mathbf{x})$. Then we define the functional derivative

$$\frac{\delta F[\rho]}{\delta \rho(\mathbf{x})} \equiv \lim_{\varepsilon \to 0} \frac{F[\rho + \varepsilon \delta_{\mathbf{x}}] - F[\rho]}{\varepsilon}$$

with

$$\delta_{\mathbf{x}}(\mathbf{y}) \equiv \delta(\mathbf{x} - \mathbf{y}) \quad \text{(Dirac's delta function)}.$$

4.1. Examples of functional differentiation

1. $\dfrac{\delta \rho(\mathbf{x})}{\delta \rho(\mathbf{y})} = \delta(\mathbf{x} - \mathbf{y})$. Indeed

$$\begin{aligned}\frac{\delta \rho(\mathbf{x})}{\delta \rho(\mathbf{y})} &= \lim_{\varepsilon \to 0} \frac{(\rho + \varepsilon \delta_{\mathbf{y}})(\mathbf{x}) - \rho(\mathbf{x})}{\varepsilon} \\ &= \delta_{\mathbf{y}}(\mathbf{x}) \\ &= \delta(\mathbf{x} - \mathbf{y}).\end{aligned}$$

2. $\frac{\delta}{\delta\rho(\mathbf{x})}\int d\mathbf{z}\, f(\mathbf{z})\,\rho(\mathbf{z}) = f(\mathbf{x})$. Indeed

$$\begin{aligned}\frac{\delta}{\delta\rho(\mathbf{x})}\int d\mathbf{z}\, f(\mathbf{z})\,\rho(\mathbf{z}) &= \lim_{\varepsilon\to 0}\frac{\int d\mathbf{z}\, f(\mathbf{z})\,(\rho+\varepsilon\delta_{\mathbf{x}})(\mathbf{z}) - \int d\mathbf{z}\, f(\mathbf{z})\,\rho(\mathbf{z})}{\varepsilon}\\ &= \lim_{\varepsilon\to 0}\frac{\int d\mathbf{z}\, f(\mathbf{z})\,\varepsilon\delta(\mathbf{x}-\mathbf{z})}{\varepsilon}\\ &= f(\mathbf{x}).\end{aligned}$$

3. $\frac{\delta}{\delta\rho(\mathbf{x})}M(\mathbf{x},\mathbf{y})\,\frac{\delta}{\delta\rho(\mathbf{y})}\int d\mathbf{u}d\mathbf{v}\,\rho(\mathbf{u})\,A(\mathbf{u},\mathbf{v})\,\rho(\mathbf{v}) = M(\mathbf{x},\mathbf{y})\,(A(\mathbf{x},\mathbf{y})+A(\mathbf{y},\mathbf{x}))$.

All rules for the common derivative also work for the functional derivative (e.g. the chain rule, product rule etc.). For instance the chain rule reads

$$\frac{\delta}{\delta\rho(\mathbf{x})} = \int d\mathbf{y}\,\frac{\delta\psi(\mathbf{y})}{\delta\rho(\mathbf{x})}\frac{\delta}{\delta\psi(\mathbf{y})}$$

when $\psi(\mathbf{y})$ is a functional of ρ.

5. Functional integration

A functional integral $\int \mathcal{D}\rho\, F[\rho]$ where F is a functional integral of ρ is defined as the integral

$$\begin{aligned}\int \mathcal{D}\rho\, F[\rho] &\equiv \int \prod_{\mathbf{x}} d\rho(\mathbf{x})\, F[\rho]\\ &\equiv \lim_{N\to\infty}\int \prod_{1\le i\le N} d\rho(\mathbf{x}_i)\, F[\rho(\mathbf{x}_1),\ldots,\rho(\mathbf{x}_N)]\end{aligned}$$

where $\{\mathbf{x}_1,\ldots,\mathbf{x}_N\}$ is a partition of the domain of ρ such that $\mathbf{x}_i\to\mathbf{x}_{i+1}$ when $N\to\infty$ and where $F[\rho(\mathbf{x}_1),\ldots,\rho(\mathbf{x}_N)]$ is a rewriting of $F[\rho]$ as a *normal function* of the N variables $\{\rho(\mathbf{x}_1),\ldots,\rho(\mathbf{x}_N)\}$ such that $F[\rho(\mathbf{x}_1),\ldots,\rho(\mathbf{x}_N)]\to F[\rho]$ when $N\to\infty$. As an example consider the functional $F[\rho]=\int dz\, f(z)\,\rho(z)$ then we can define

$$F[\rho(x_1),\ldots,\rho(x_{N-1})] = \sum_{1\le i\le N-1} f(x_i)\,\rho(x_i)\,(x_{i+1}-x_i)$$

a Riemann sum approximation of the integral $\int dz\, f(z)\,\rho(z)$ (where $x_i\to x_{i+1}$ when $N\to\infty$) and $F[\rho(x_1),\ldots,\rho(x_{N-1})]$ is then a normal function of the $N-1$ *variables* $\rho(x_i)$.

6. Gaussian functional integrals

In what follows we want to calculate the functional integral

$$I \equiv \int \mathcal{D}\rho \, \exp\left[-\frac{1}{2}\int d\mathbf{x}d\mathbf{y}\,\rho\left(\mathbf{x}\right)K\left(\mathbf{x},\mathbf{y}\right)\rho\left(\mathbf{y}\right) - i\int d\mathbf{x}\,L\left(\mathbf{x}\right)\rho\left(\mathbf{x}\right)\right]F\left[\rho\right] \tag{4}$$

where $L\left(\mathbf{x}\right)$ is a given function of $\mathbf{x}$ and where $K\left(\mathbf{x},\mathbf{y}\right)$ is an invertible (not necessarily hermitian) integral operator.

To this end we use an identity of W. Siegel (Siegel, 2005) (since $f\left(x+y\right) = e^{x\partial_y}f\left(y\right)$) and use equation (3)

$$\begin{aligned}
\int_{-\infty}^{\infty} d^n u \, \exp\left[-\frac{1}{2}u^t K u\right] f\left(u\right) &= \int_{-\infty}^{\infty} d^n u \, \exp\left[-\frac{1}{2}u^t \mathcal{K} u\right] f\left(u+v\right) \text{ at } v=0 \\
&= \int_{-\infty}^{\infty} d^n u \, \exp\left[-\frac{1}{2}u^t \mathcal{K} u + u^t\frac{\partial}{\partial v}\right] f\left(v\right) \text{ at } v=0 \\
&= C\frac{1}{\sqrt{\det\mathcal{K}}}\exp\left[\frac{1}{2}\left(\frac{\partial}{\partial v}\right)^t \mathcal{K}^{-1}\frac{\partial}{\partial v}\right] f\left(v\right) \text{ at } v=0 \\
\mathcal{K} &= \frac{1}{2}\left(K+K^t\right)
\end{aligned}$$

since $u^tKu = \frac{1}{2}u^tKu + \frac{1}{2}u^tK^tu$ where $u = \left(u_1,\ldots,u_n\right)$, $v = \left(v_1,\ldots,v_n\right)$, $\frac{\partial}{\partial v} = \left(\frac{\partial}{\partial v_1},\ldots,\frac{\partial}{\partial v_n}\right)$ and K is an $n\times n$ invertible (and in our case complex) matrix. (Actually u is the column vector $\begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix}$ and $u^t = \left(u_1,\ldots,u_n\right)$ etc.) (we also used (3)). The continuous version of the above identity is then

$$\begin{aligned}
&\int \mathcal{D}\rho \, \exp\left[-\frac{1}{2}\int d\mathbf{x}d\mathbf{y}\,\rho\left(\mathbf{x}\right)K_{\mathbf{x},\mathbf{y}}\rho\left(\mathbf{y}\right)\right]F\left[\rho\right] \\
&\qquad = C\frac{1}{\sqrt{\det\mathcal{K}}}\exp\left[\frac{1}{2}\int d\mathbf{x}d\mathbf{y}\,\frac{\delta}{\delta\rho\left(\mathbf{x}\right)}\mathcal{K}^{-1}_{\mathbf{x},\mathbf{y}}\frac{\delta}{\delta\rho\left(\mathbf{y}\right)}\right]F\left[\rho\right]\Big|_{\rho=0}
\end{aligned} \tag{5}$$

where we used (and possibly later will use) several notational conventions

$$\begin{aligned}
K_{\mathbf{x},\mathbf{y}} &= K\left(\mathbf{x},\mathbf{y}\right) \\
K^{-1}_{\mathbf{x},\mathbf{y}} &= \left(K^{-1}\right)_{\mathbf{x},\mathbf{y}} \\
\rho^t K \rho &= \int d\mathbf{x}d\mathbf{y}\,\rho\left(\mathbf{x}\right)K_{\mathbf{x},\mathbf{y}}\rho\left(\mathbf{y}\right) \\
L^t\rho &= \int d\mathbf{x}\,L\left(\mathbf{x}\right)\rho\left(\mathbf{x}\right)
\end{aligned} \tag{6}$$

Next consider the functional integral I (4). We shift (change of variable) $\rho \to \rho - \varphi$. That is

$$
\begin{aligned}
\rho(\mathbf{x}) &\to \rho(\mathbf{x}) - \varphi(\mathbf{x}) \\
d\rho(\mathbf{x}) &\to d(\rho(\mathbf{x}) - \varphi(\mathbf{x})) = d\rho(\mathbf{x}) \\
\text{thus } \mathcal{D}\rho &\to \mathcal{D}\rho
\end{aligned}
$$

With this "translation" we can write

$$
\begin{aligned}
I = & \int \mathcal{D}\rho \, \exp\left[-\frac{1}{2}\rho^t \mathcal{K}\rho - iL^t\rho\right] F[\rho] \\
= & \int \mathcal{D}\rho \, \exp\left[-\frac{1}{2}(\rho+\varphi)^t \mathcal{K}(\rho+\varphi) - iL^t(\rho+\varphi)\right] F[\rho+\varphi] \\
= & \int \mathcal{D}\rho \, \exp\left[-\frac{1}{2}\rho^t \mathcal{K}\rho - \frac{1}{2}\rho^t\mathcal{K}\varphi - \frac{1}{2}\varphi^t\mathcal{K}^t\rho - iL^t\rho\right] F[\rho+\varphi] \\
& \times \exp\left[-\frac{1}{2}\varphi^t\mathcal{K}\varphi - iL^t\varphi\right] \\
= & \int \mathcal{D}\rho \, \exp\left[-\frac{1}{2}\rho^t \mathcal{K}\rho - \frac{1}{2}\rho^t\left(\mathcal{K}\varphi + \mathcal{K}^t\varphi + 2iL\right)\right] F[\rho+\varphi] \\
& \times \exp\left[-\frac{1}{2}\varphi^t K\varphi - iL^t\varphi\right] \\
= & \int \mathcal{D}\rho \, \exp\left[-\frac{1}{2}\rho^t \mathcal{K}\rho\right] F[\rho+\varphi_0] \times \exp\left[-\frac{1}{2}L^t\mathcal{K}^{-1}L\right] \\
& \text{ if } \varphi_0 = -i\mathcal{K}^{-1}L \\
= & \, C\frac{1}{\sqrt{\det\mathcal{K}}} \exp\left[\frac{1}{2}\int \frac{\delta}{\delta\rho(\mathbf{x})}\mathcal{K}^{-1}_{\mathbf{x},\mathbf{y}}\frac{\delta}{\delta\rho(\mathbf{y})}\right] F[\rho+\varphi_0]\Big|_{\rho=0} \\
& \times \exp\left[-\frac{1}{2}L^t\mathcal{K}^{-1}L\right] \quad \text{where we use eq. (5)} \\
= & \, C\frac{1}{\sqrt{\det\mathcal{K}}} \exp\left[-\frac{1}{2}L^t\mathcal{K}^{-1}L\right] \times \exp\left[\frac{1}{2}\int \frac{\delta}{\delta\varphi(\mathbf{x})}\mathcal{K}^{-1}_{\mathbf{x},\mathbf{y}}\frac{\delta}{\delta\varphi(\mathbf{y})}\right] F[\varphi]\Big|_{\varphi=\varphi_0}
\end{aligned}
$$

In the above derivations we used the identities

$$
\begin{aligned}
L^t\rho &= \rho^t L \\
\varphi^t K\rho &= (K\rho)^t\varphi \\
&= \rho^t K^t\varphi \\
\frac{\delta}{\delta\rho(\mathbf{x})}\Phi[\rho+\varphi_0]\Big|_{\rho=0} &= \frac{\delta}{\delta\varphi(\mathbf{x})}\Phi[\varphi]\Big|_{\varphi=\varphi_0}
\end{aligned}
$$

So we recap

$$\int \mathcal{D}\rho \, \exp\left[-\frac{1}{2}\int d\mathbf{x}d\mathbf{y}\, \rho\left(\mathbf{x}\right) K\left(\mathbf{x},\mathbf{y}\right)\rho\left(\mathbf{y}\right) - i\int d\mathbf{x}\, L\left(\mathbf{x}\right)\rho\left(\mathbf{x}\right)\right] F\left[\rho\right]$$
$$= C\frac{1}{\sqrt{\det\mathcal{K}}}\exp\left[-\frac{1}{2}L^t\mathcal{K}^{-1}L\right]\times\exp\left[\frac{1}{2}\int\frac{\delta}{\delta\varphi\left(\mathbf{x}\right)}\mathcal{K}^{-1}_{\mathbf{x},\mathbf{y}}\frac{\delta}{\delta\varphi\left(\mathbf{y}\right)}\right]F\left[\varphi\right]\Big|_{\varphi=\varphi_0}$$
$$\text{where } \varphi_0 = -i\mathcal{K}^{-1}L \quad (7)$$

7. A general scheme for calculating more general functional integrals.

Suppose we want to calculate the functional integral

$$I = \int \mathcal{D}\phi\, \exp\left[-\frac{1}{2}\int\phi K\phi\right] H\left[\phi\right]\Psi\left[\phi\right].$$

We now know that the integral I equals (up to an unimportant constant) with $\mathcal{K} = \frac{1}{2}\left(K + K^t\right)$

$$I = \frac{1}{\sqrt{\det\mathcal{K}}}\exp\left[\frac{1}{2}\int\frac{\delta}{\delta\phi}\mathcal{K}^{-1}\frac{\delta}{\delta\phi}\right]H\left[\phi\right]\Psi\left[\phi\right]\Big|_{\phi=0}.$$

We now want to separate the differentations on $H\left[\phi\right]$ and $\Psi\left[\phi\right]$. To do this we remark that (see)

$$f\left(\partial_x\right)g\left(x, x+y\right) = f\left(\partial_x^{'} + \partial_y^{'}\right)g\left(x', y'\right)\ \ x' = x,\ y' = x+y$$

evaluated at $x = y = 0$. Using this identity we can rewrite I as (up to a constant)

$$\begin{aligned} I &= \frac{1}{\sqrt{\det\mathcal{K}}}\exp\left[\int\frac{1}{2}\frac{\delta}{\delta\phi}\mathcal{K}^{-1}\frac{\delta}{\delta\phi} + \frac{\delta}{\delta\phi}\mathcal{K}^{-1}\frac{\delta}{\delta\varphi} + \right. \\ & \left.\frac{1}{2}\frac{\delta}{\delta\varphi}\mathcal{K}^{-1}\frac{\delta}{\delta\varphi}\right]H\left[\phi\right]\Psi\left[\phi\right]\Big|_{\phi=\varphi=0}. \end{aligned}$$

That is

$$I = \frac{1}{\sqrt{\det\mathcal{K}}}\exp\left[\frac{1}{2}\int\frac{\delta}{\delta\phi}\mathcal{K}^{-1}\frac{\delta}{\delta\varphi}\right]Z\left[\phi\right]\Delta\left[\varphi\right]\Big|_{\phi=\varphi=0} \quad (8)$$

where

$$\begin{aligned} Z\left[\phi\right] &= \exp\left[\frac{1}{2}\int\frac{\delta}{\delta\phi}\mathcal{K}^{-1}\frac{\delta}{\delta\phi}\right]H\left[\phi\right] \\ \Delta\left[\varphi\right] &= \exp\left[\frac{1}{2}\frac{\delta}{\delta\varphi}\mathcal{K}^{-1}\frac{\delta}{\delta\varphi}\right]\Psi\left[\varphi\right] \end{aligned} \quad (9)$$

8. The expectation value of the triplet in $P1$

We want to calculate the functional integral (P is the known Patterson function)

$$I \equiv Cte \int \mathcal{D}\rho\, \delta\left(\rho^2 - \frac{\delta\left(\mathbf{0}\right)}{\sqrt{N}}\rho\right) \times \prod_{\mathbf{x}} \delta\left(\int d\mathbf{y}\, \rho\left(\mathbf{y}\right) \rho\left(\mathbf{x}+\mathbf{y}\right) - P\left(\mathbf{x}\right)\right) \delta\left(\int \rho - \sqrt{N}\right) \times \int d\mathbf{x} d\mathbf{u} d\mathbf{v}\, \rho\left(\mathbf{x}\right) \rho\left(\mathbf{x}+\mathbf{u}\right) \rho\left(\mathbf{x}+\mathbf{v}\right) \exp\left[2\pi i\left(\mathbf{h}\cdot\mathbf{u}+\mathbf{k}\cdot\mathbf{v}\right)\right] \quad (10)$$

The measure

$$\delta\left(\rho^2 - \frac{\delta\left(\mathbf{0}\right)}{\sqrt{N}}\rho\right) \prod_{\mathbf{x}} \delta\left(\int d\mathbf{y}\, \rho\left(\mathbf{y}\right) \rho\left(\mathbf{x}+\mathbf{y}\right) - P\left(\mathbf{x}\right)\right) \delta\left(\int \rho - \sqrt{N}\right) \quad (11)$$

is (apart from a normalization constant) a positive uniform measure on the space of all distributions ρ on the unit cell in $P1$. Clearly

$$E_{\mathbf{h}} E_{\mathbf{k}} E_{-\mathbf{h}-\mathbf{k}}\left[\rho\right] \equiv \int d\mathbf{x} d\mathbf{u} d\mathbf{v}\, \rho\left(\mathbf{x}\right) \rho\left(\mathbf{x}+\mathbf{u}\right) \rho\left(\mathbf{x}+\mathbf{v}\right) \exp\left[2\pi i\left(\mathbf{h}\cdot\mathbf{u}+\mathbf{k}\cdot\mathbf{v}\right)\right]$$

is nothing else but the triplet $E_{\mathbf{h}} E_{\mathbf{k}} E_{-\mathbf{h}-\mathbf{k}}$ expressed as a functional of ρ. So

$$I = \left\langle E_{\mathbf{h}} E_{\mathbf{k}} E_{-\mathbf{h}-\mathbf{k}}\left[\rho\right]\right\rangle$$

is the expectation value of the triplet where we average over the electronic distributions ρ of the unit cell.

$$\delta\left(\rho^2 - \frac{\delta\left(\mathbf{0}\right)}{\sqrt{N}}\rho\right)$$

is a delta functional constraint expressing the fact that for every $\mathbf{x}$, $\rho\left(\mathbf{x}\right)$ is either zero or equals a peak of "strength" $\frac{\delta(\mathbf{0})}{\sqrt{N}}$. Together with the condition

$$\delta\left(\int \rho - \sqrt{N}\right)$$

we express the fact that ρ is a sum of N equal atoms of *strength* $\frac{\delta(\mathbf{0})}{\sqrt{N}}$.

Finally the last constraint

$$\prod_{\mathbf{x}} \delta \left(\int d\mathbf{y}\, \rho\left(\mathbf{y}\right) \rho\left(\mathbf{x}+\mathbf{y}\right) - P\left(\mathbf{x}\right) \right)$$

expresses the fact that ρ is a solution of the phase problem. Remark also that the constant of normalization Cte equals

$$Cte^{-1} = \int \mathcal{D}\rho\, \delta \left(\rho^2 - \frac{\delta\left(\mathbf{0}\right)}{\sqrt{N}} \rho \right) \times \\ \prod_{\mathbf{x}} \delta \left(\int d\mathbf{y}\, \rho\left(\mathbf{y}\right) \rho\left(\mathbf{x}+\mathbf{y}\right) - P\left(\mathbf{x}\right) \right) \delta \left(\int \rho - \sqrt{N} \right).$$

Next we write the delta functions as Fourier integrals up to a constant

$$\begin{aligned} \delta \left(\rho^2 - \frac{\delta\left(\mathbf{0}\right)}{\sqrt{N}} \rho \right) &= \int \mathcal{D}\mu\, \exp \left[i \int d\mathbf{x}\, \mu\left(\mathbf{x}\right) \left(\rho^2\left(\mathbf{x}\right) - \frac{\delta\left(\mathbf{0}\right)}{\sqrt{N}} \right) \right] \\ \prod_{\mathbf{x}} \delta \left(\int d\mathbf{y}\, \rho\left(\mathbf{y}\right) \rho\left(\mathbf{x}+\mathbf{y}\right) - P\left(\mathbf{x}\right) \right) &= \int \mathcal{D}\lambda\, \exp \left[i \int d\mathbf{x}\, \lambda\left(\mathbf{x}\right) \times \right. \\ & \qquad \left. \left(\int d\mathbf{y}\, \rho\left(\mathbf{y}\right) \rho\left(\mathbf{x}+\mathbf{y}\right) - P\left(\mathbf{x}\right) \right) \right] \\ \delta \left(\int \rho - \sqrt{N} \right) &= \int d\kappa\, \exp \left[i\kappa \left(\int \rho - \sqrt{N} \right) \right] \end{aligned}$$

So eventually we can express I up to a constant as the functional integral (except $\int d\kappa$ which is a normal integral)

$$I = \int d\kappa \int \mathcal{D}\lambda \mathcal{D}\mu \mathcal{D}\rho\, \exp \left[i \int d\mathbf{x} d\mathbf{y}\, \rho\left(\mathbf{x}\right) \lambda\left(\mathbf{x}-\mathbf{y}\right) \rho\left(\mathbf{y}\right) + \right. \\ i \int d\mathbf{x}\, \mu\left(\mathbf{x}\right) \rho^2\left(\mathbf{x}\right) - i \frac{\delta\left(\mathbf{0}\right)}{\sqrt{N}} \int d\mathbf{x}\, \mu\left(\mathbf{x}\right) \rho\left(\mathbf{x}\right) + i\kappa \int d\mathbf{x}\, \rho\left(\mathbf{x}\right) - \\ \left. i \int d\mathbf{x}\, \lambda\left(\mathbf{x}\right) P\left(\mathbf{x}\right) - i\kappa\sqrt{N} \right] E_{\mathbf{h}} E_{\mathbf{k}} E_{-\mathbf{h}-\mathbf{k}} \left[\rho\right]$$

This can also be written more compactly as

$$I = \int d\kappa \int \mathcal{D}\lambda \mathcal{D}\mu \mathcal{D}\rho\, \exp \left[i\rho^t \left(M + \mathcal{L}\right) \rho - \right. \\ \left. i \left(\frac{\delta\left(\mathbf{0}\right)}{\sqrt{N}} \mu^t - \kappa \right) \rho - i\lambda^t P - i\kappa\sqrt{N} \right] E_{\mathbf{h}} E_{\mathbf{k}} E_{-\mathbf{h}-\mathbf{k}} \left[\rho\right] \quad (12)$$

where

$$\begin{aligned}
\mu^t\rho &= \int d\mathbf{x}\,\mu(\mathbf{x})\,\rho(\mathbf{x}) \\
M_{\mathbf{x},\mathbf{y}} &= \mu(\mathbf{x})\,\delta(\mathbf{x}-\mathbf{y}) \\
\mathcal{L} &= \frac{1}{2}\left(L+L^t\right) \\
L_{\mathbf{x},\mathbf{y}} &= \lambda(\mathbf{x}-\mathbf{y})
\end{aligned} \tag{13}$$

Remark that L is not symmetric.

9. Doing the $\mathcal{D}\rho$ integration

It follows from (12 in section (1)) that (up to a constant) and *after* the transformation $\mu \to \frac{\sqrt{N}}{\delta(\mathbf{0})}(\mu+\kappa)$ (in which case $\mathcal{D}\mu \to Cte\mathcal{D}\mu$ and we discard the unimportant constant)

$$\begin{aligned}
I = \int_{-\infty}^{\infty} d\kappa e^{-i\kappa\sqrt{N}} \int \mathcal{D}\lambda\mathcal{D}\mu \frac{1}{\sqrt{\det\bar{\mathcal{K}}}} \exp\left[-\frac{1}{2}\mu^t\bar{\mathcal{K}}^{-1}\mu - i\lambda^t P\right] \times \\
\exp\left[\frac{1}{2}\frac{\delta}{\delta\rho}^t\bar{\mathcal{K}}^{-1}\frac{\delta}{\delta\rho}\right] E_{\mathbf{h}}E_{\mathbf{k}}E_{-\mathbf{h}-\mathbf{k}}[\rho]\Big|_{\rho=\varphi}
\end{aligned} \tag{14}$$

where

$$\begin{aligned}
\bar{\mathcal{K}} &= -2i\left(\mathcal{L} + \frac{\sqrt{N}(M+\kappa)}{\delta(\mathbf{0})}\right) \\
\varphi &= -i\bar{\mathcal{K}}^{-1}\mu \\
&= \frac{1}{2}\left(\mathcal{L} + \frac{\sqrt{N}(M+\kappa)}{\delta(\mathbf{0})}\right)^{-1}\mu \\
\mathcal{L} &= \frac{L+L^t}{2}
\end{aligned}$$

Next since $\mathrm{Tr}A = \int d\mathbf{x}\, A_{\mathbf{x},\mathbf{x}}$ and $\int_{\text{unit cell}} d\mathbf{x} = 1$ and $\lambda(\mathbf{0}) = \int d\mathbf{x}\,\lambda(\mathbf{x})\,\delta(\mathbf{x})$ and $\delta(\mathbf{0})$ is an infinite number and since $\det\bar{\mathcal{K}} = \exp\left(\mathrm{Tr}\ln\bar{\mathcal{K}}\right)$ we have

$$
\begin{aligned}
\frac{1}{\sqrt{\det\bar{\mathcal{K}}}} &= Cte\,\exp\left\{-\frac{1}{2}\mathrm{Tr}\ln\left[-i\left(\mathcal{L}+\frac{\sqrt{N}\left(M+\kappa\right)}{\delta\left(\mathbf{0}\right)}\right)\right]\right\}\\
&= Cte\,\exp\left\{-\frac{1}{2}\mathrm{Tr}\ln\left[1-i\left(\left(\mathcal{L}-i\right)+\frac{\sqrt{N}\left(M+\kappa\right)}{\delta\left(\mathbf{0}\right)}\right)\right]\right\}\\
&= Cte\,\exp\left[\frac{i}{2}\mathrm{Tr}\mathcal{L}+\frac{i}{2}\mathrm{Tr}\frac{\left(M+\kappa\right)\sqrt{N}}{\delta\left(\mathbf{0}\right)}+\right.\\
&\qquad\left.\left(-\frac{1}{2}\right)^{2}\left(-i\right)^{2}\mathrm{Tr}\left(\left(\mathcal{L}-i\right)+\frac{\sqrt{N}\left(M+\kappa\right)}{\delta\left(\mathbf{0}\right)}\right)^{2}+O\left(\left\{\lambda,\mu\right\}^{3}\right)\right]\\
&\propto \exp\left[i\int d\mathbf{x}\,\lambda\left(\mathbf{x}\right)\delta\left(\mathbf{x}\right)+i\sqrt{N}\int\left(\mu+\kappa\right)-\frac{1}{8}\lambda^{t}\left(1+\Sigma\right)\lambda-\right.\\
&\qquad\left.\frac{\sqrt{N}}{2\delta\left(\mathbf{0}\right)}\lambda\left(\mathbf{0}\right)\int\left(\mu+\kappa\right)-\frac{N}{4\delta\left(\mathbf{0}\right)}\left(\int\mu^{2}+2\kappa\int\mu+\kappa^{2}\right)\right.\\
Cte &= \frac{1}{\sqrt{\det\left(2\right)}}\\
\Sigma f\left(\mathbf{x}\right) &= f\left(-\mathbf{x}\right)
\end{aligned}
\tag{15}
$$

Indeed

$$
\begin{aligned}
-\frac{1}{4}\mathrm{Tr}\left(\mathcal{L}-i\right)^{2} &= -\frac{1}{8}\lambda^{t}\left(1+\Sigma\right)\lambda+\frac{i}{2}\lambda\left(\mathbf{0}\right)+Cte\\
\frac{i}{2}\mathrm{Tr}\frac{\sqrt{N}\left(M+\kappa\right)}{\delta\left(\mathbf{0}\right)} &= \frac{i}{2}\frac{\sqrt{N}}{\delta\left(\mathbf{0}\right)}\delta\left(\mathbf{0}\right)\int\left(\mu+\kappa\right)=i\frac{\sqrt{N}}{2}\int\left(\mu+\kappa\right)\\
2\left(-\frac{1}{4}\right)\mathrm{Tr}\left(\mathcal{L}-i\right)\frac{\sqrt{N}\left(M+\kappa\right)}{\delta\left(\mathbf{0}\right)} &= -\lambda\left(\mathbf{0}\right)\frac{\sqrt{N}}{2\delta\left(\mathbf{0}\right)}\int\left(\mu+\kappa\right)+\frac{i}{2}\sqrt{N}\int\left(\mu+\kappa\right)\\
\mathrm{Tr}L^{2} &= \int d\mathbf{x}d\mathbf{y}\,\lambda\left(\mathbf{x}-\mathbf{y}\right)\lambda\left(\mathbf{y}-\mathbf{x}\right)=\lambda^{t}\Sigma\lambda\\
\mathrm{Tr}LL^{t} &= \int\lambda^{2}\\
-\frac{1}{4}\mathrm{Tr}\left(\frac{\sqrt{N}\left(M+\kappa\right)}{\delta\left(\mathbf{0}\right)}\right)^{2} &= -\frac{N}{4\delta\left(\mathbf{0}\right)^{2}}\delta\left(\mathbf{0}\right)\int\left(\mu+\kappa\right)^{2}\\
&= -\frac{N}{4\delta\left(\mathbf{0}\right)}\int\mu^{2}-\frac{1}{2}\frac{N\kappa}{\delta\left(\mathbf{0}\right)}\int\mu-\frac{N}{4\delta\left(\mathbf{0}\right)}\kappa^{2}
\end{aligned}
$$

We now do a change of variable $\kappa \to \frac{\sqrt{\delta(\mathbf{0})}}{\sqrt{N}}\kappa$. Putting then (15) into (14) we obtain for I

$$
\begin{aligned}
I = & \int_{-\infty}^{\infty} d\kappa \exp\left[-\frac{1}{4}\kappa^2\right] \int \mathcal{D}\lambda\mathcal{D}\mu \times \\
& \exp\left[-\frac{1}{2}\mu^t \left(-2i\left(\mathcal{L} + \frac{M\sqrt{N}}{\delta\left(\mathbf{0}\right)} + \frac{\kappa}{\sqrt{\delta\left(\mathbf{0}\right)}}\right)\right)^{-1} \mu - i\lambda^t \left(Q - i\frac{\kappa}{2\sqrt{\delta\left(\mathbf{0}\right)}}\delta\right)\right] \times \\
& \exp\left[-i\mu^t\sqrt{N}\left(-1 - i\frac{\kappa}{2\sqrt{\delta\left(\mathbf{0}\right)}} - i\lambda\left(\mathbf{0}\right)\frac{\sqrt{N}}{2\delta\left(\mathbf{0}\right)}\right) - \frac{1}{8}\lambda^t\left(1+\Sigma\right)\lambda\right] \times \\
& \exp\left[\frac{1}{2}\frac{\delta}{\delta\rho}^t \left(-2i\left(\mathcal{L} + \frac{M\sqrt{N}}{\delta\left(\mathbf{0}\right)} + \frac{\kappa}{\sqrt{\delta\left(\mathbf{0}\right)}}\right)\right)^{-1} \frac{\delta}{\delta\rho}\right] E_{\mathbf{h}}E_{\mathbf{k}}E_{-\mathbf{h}-\mathbf{k}}\left[\rho\right]\Bigg|_{\rho=\varphi} \\
& + O\left(\delta\left(\mathbf{0}\right)^{-1}\right)
\end{aligned}
$$

$$Q = P - \delta \tag{16}$$

$$
\begin{aligned}
\varphi &= -i\mathcal{K}^{-1}\mu \\
\mathcal{K} &= -2i\left(\mathcal{L} + \frac{M\sqrt{N}}{\delta\left(\mathbf{0}\right)} + \frac{\kappa}{\sqrt{\delta\left(\mathbf{0}\right)}}\right)
\end{aligned} \tag{17}
$$

We now use the identity (Siegel, 2005)

$$\frac{1}{A+B} = \frac{1}{A} - \frac{1}{A}B\frac{1}{A} + \ldots$$

to develop $\left(A - 2i\frac{M\sqrt{N}}{\delta(\mathbf{0})}\right)^{-1}$,

$$
\begin{aligned}
\left(A - 2i\frac{M\sqrt{N}}{\delta\left(\mathbf{0}\right)}\right)^{-1} &= \frac{1}{A} + 2i\frac{1}{A}\frac{M\sqrt{N}}{\delta\left(\mathbf{0}\right)}\frac{1}{A} + O\left(\delta\left(\mathbf{0}\right)^{-2}\right) \\
A &= -2i\left(\mathcal{L} + \frac{\kappa}{\sqrt{\delta\left(\mathbf{0}\right)}}\right)
\end{aligned}
$$

Then

$$
\begin{aligned}
I &= \int_{-\infty}^{\infty} d\kappa \exp\left[-\frac{1}{4}\kappa^2\right] \int \mathcal{D}\lambda\mathcal{D}\mu \ \times \\
&\quad \exp\left[-\frac{1}{2}\mu^t A^{-1}\mu - i\lambda^t\left(Q - i\frac{\kappa}{2\sqrt{\delta\left(\mathbf{0}\right)}}\delta\right)\right] \times \\
&\quad \exp\left[-i\mu^t\sqrt{N}\left(-1 - \frac{i\kappa}{2\sqrt{\delta\left(\mathbf{0}\right)}} - i\lambda\left(\mathbf{0}\right)\frac{\sqrt{N}}{2\delta\left(\mathbf{0}\right)}\right) - \frac{1}{8}\lambda^t\left(1+\Sigma\right)\lambda\right] \times \\
&\quad \exp\left[i\mu^t\frac{1}{A}\frac{M\sqrt{N}}{\delta\left(\mathbf{0}\right)}\frac{1}{A}\mu\right] \\
&\quad \exp\left[\frac{1}{2}\frac{\delta}{\delta\rho}^t\mathcal{K}^{-1}\frac{\delta}{\delta\rho}\right] E_{\mathbf{h}}E_{\mathbf{k}}E_{-\mathbf{h}-\mathbf{k}}\left[\rho\right]_{\rho=\varphi} \\
Q &= P - \delta \qquad (18) \\
\varphi &= -i\mathcal{K}^{-1}\mu \\
\mathcal{K} &= -2i\left(\mathcal{L} + \frac{\kappa}{\sqrt{\delta\left(\mathbf{0}\right)}} + \frac{M\sqrt{N}}{\delta\left(\mathbf{0}\right)}\right) \\
&= A - 2i\frac{M\sqrt{N}}{\delta\left(\mathbf{0}\right)} \qquad (19)
\end{aligned}
$$

Finally we calculate

$$
\begin{aligned}
&\exp\left[\frac{1}{2}\frac{\delta}{\delta\rho}^t\mathcal{K}^{-1}\frac{\delta}{\delta\rho}\right] E_{\mathbf{h}}E_{\mathbf{k}}E_{-\mathbf{h}-\mathbf{k}}\left[\rho\right]\Big|_{\rho=\varphi} \\
&\qquad \equiv \exp\left[\frac{1}{2}\int d\mathbf{x}d\mathbf{y}\,\frac{\delta}{\delta\rho\left(\mathbf{x}\right)}\mathcal{K}^{-1}_{\mathbf{x},\mathbf{y}}\frac{\delta}{\delta\rho\left(\mathbf{y}\right)}\right] E_{\mathbf{h}}E_{\mathbf{k}}E_{-\mathbf{h}-\mathbf{k}}\left[\rho\right]\Big|_{\rho=\varphi} \\
&= E_{\mathbf{h}}E_{\mathbf{k}}E_{-\mathbf{h}-\mathbf{k}}\left[\rho\right]\big|_{\rho=-i\mathcal{K}^{-1}\mu} - \\
&\quad i\int d\mathbf{u}d\mathbf{v}\,\exp\left[2\pi i\left(\mathbf{h}\cdot\mathbf{u}+\mathbf{k}\cdot\mathbf{v}\right)\right]\left[\int d\mathbf{z}d\mathbf{y}\,\mathcal{K}^{-1}_{\mathbf{z},\mathbf{z}+\mathbf{u}}\mathcal{K}^{-1}_{\mathbf{z}+\mathbf{v},\mathbf{y}}\mu\left(\mathbf{y}\right) + \right. \\
&\qquad \left. \int d\mathbf{z}d\mathbf{y}\,\mathcal{K}^{-1}_{\mathbf{z},\mathbf{z}+\mathbf{v}}\mathcal{K}^{-1}_{\mathbf{z}+\mathbf{u},\mathbf{y}}\mu\left(\mathbf{y}\right) + \int d\mathbf{z}d\mathbf{y}\,\mathcal{K}^{-1}_{\mathbf{z}+\mathbf{u},\mathbf{z}+\mathbf{v}}\mathcal{K}^{-1}_{\mathbf{z},\mathbf{y}}\mu\left(\mathbf{y}\right)\right]
\end{aligned}
$$

10. Doing the $\mathcal{D}\mu$ integration

First we calculate

$$\begin{aligned}
\frac{1}{\sqrt{\det A^{-1}}} &= \sqrt{\det A} \\
&= \sqrt{\det\left(-2i\right)\det\left(\mathcal{L}+\frac{\kappa}{\sqrt{\delta\left(\mathbf{0}\right)}}\right)} \\
&\propto \sqrt{\det\left(\mathcal{L}+\frac{\kappa}{\sqrt{\delta\left(\mathbf{0}\right)}}\right)} \\
&\propto \exp\left[\frac{1}{2}\mathrm{Tr}\ln\left(1+\left(\mathcal{L}-1\right)+\frac{\kappa}{\sqrt{\delta\left(\mathbf{0}\right)}}\right)\right] \\
&\propto \exp\left[-\frac{1}{8}\lambda^t\left(1+\Sigma\right)\lambda-\frac{1}{4}\kappa^2+\lambda^t\delta+\kappa\sqrt{\delta\left(\mathbf{0}\right)}-\frac{\kappa}{2\sqrt{\delta\left(\mathbf{0}\right)}}\lambda^t\delta\right]
\end{aligned}$$

Next we can do, from (19) and the usual rules for calculating a gaussian integral, the $\mathcal{D}\mu$-integration. We get

$$\begin{aligned}
I &= \int d\kappa\,\exp\left[\kappa\sqrt{\delta\left(\mathbf{0}\right)}-\frac{1}{2}\kappa^2\right]\int\mathcal{D}\lambda\,\exp\left[-\frac{1}{4}\lambda^t\left(1+\Sigma\right)\lambda-i\lambda^t\left(Q+i\delta-i\frac{\kappa}{\sqrt{\delta\left(\mathbf{0}\right)}}\delta\right)\right]\times \\
&\quad \exp\left[iN\left(\lambda^t+\frac{\kappa}{\sqrt{\delta\left(\mathbf{0}\right)}}\right)\left(1+i\frac{\kappa}{2\sqrt{\delta\left(\mathbf{0}\right)}}+\lambda\left(\mathbf{0}\right)\frac{\sqrt{N}}{2\delta\left(\mathbf{0}\right)}\right)^2\right]\times \\
&\quad \exp\left[\frac{1}{2}\frac{\delta}{\delta\mu}^t A\frac{\delta}{\delta\mu}\right]H\left[\mu\right]\mathcal{H}\left[\mu\right]_{\mu=\phi} \\
\phi &= iA\sqrt{N}\left(1+i\frac{\kappa}{2\sqrt{\delta\left(\mathbf{0}\right)}}+i\lambda\left(\mathbf{0}\right)\frac{\sqrt{N}}{2\delta\left(\mathbf{0}\right)}\right) \\
A &= -2i\left(\mathcal{L}+\frac{\kappa}{\sqrt{\delta\left(\mathbf{0}\right)}}\right) \\
\mathcal{H}\left[\mu\right] &= \exp\left[i\mu^t\frac{1}{A}\frac{M\sqrt{N}}{\delta\left(\mathbf{0}\right)}\frac{1}{A}\mu\right] \\
H\left[\mu\right] &= \left.E_{\mathbf{h}}E_{\mathbf{k}}E_{-\mathbf{h}-\mathbf{k}}\left[\rho\right]\right|_{\rho=-i\mathcal{K}^{-1}\mu}- \\
&\quad i\int d\mathbf{u}d\mathbf{v}\,\exp\left[2\pi i\left(\mathbf{h}\cdot\mathbf{u}+\mathbf{k}\cdot\mathbf{v}\right)\right]\left[\int d\mathbf{z}d\mathbf{y}\,\mathcal{K}^{-1}_{\mathbf{z},\mathbf{z}+\mathbf{u}}\mathcal{K}^{-1}_{\mathbf{z}+\mathbf{v},\mathbf{y}}\mu\left(\mathbf{y}\right)+\right. \\
&\quad \int d\mathbf{z}d\mathbf{y}\,\mathcal{K}^{-1}_{\mathbf{z},\mathbf{z}+\mathbf{v}}\mathcal{K}^{-1}_{\mathbf{z}+\mathbf{u},\mathbf{y}}\mu\left(\mathbf{y}\right)+\int d\mathbf{z}d\mathbf{y}\,\mathcal{K}^{-1}_{\mathbf{z}+\mathbf{u},\mathbf{z}+\mathbf{v}}\mathcal{K}^{-1}_{\mathbf{z},\mathbf{y}}\mu\left(\mathbf{y}\right) \qquad (20)
\end{aligned}$$

Next it is time to diagonalize $\mathcal{L}$. It is easy to do this with bra ket notation. We define the ket $|\mathbf{h}\rangle$ as the function

$$< \mathbf{x}|\mathbf{h} >= \exp\left[-2\pi i\mathbf{h}\cdot\mathbf{x}\right]$$

and thus

$$\begin{aligned} \langle\mathbf{h}|\mathbf{x}\rangle &\equiv \overline{< \mathbf{x}|\mathbf{h} >} \\ &= < -\mathbf{x}|\mathbf{h} > \\ &= < \mathbf{x}| - \mathbf{h} > \end{aligned}$$

And we use the following identities

$$\begin{aligned} \mathrm{Id} &= \int d\mathbf{x}\ |\mathbf{x}\rangle\langle\mathbf{x}| \\ < \mathbf{x}|\mathbf{y} > &= \delta\left(\mathbf{x}-\mathbf{y}\right) \\ \hat{\lambda}\left(\mathbf{q}\right) \equiv < \mathbf{q}|\lambda > &= \int d\mathbf{x}\ < \mathbf{q}|\mathbf{x} >< \mathbf{x}|\lambda > \\ &= \int d\mathbf{x}\,\lambda\left(\mathbf{x}\right)\exp\left[2\pi i\mathbf{q}\cdot\mathbf{x}\right] \\ \lambda\left(\mathbf{x}\right) &= \left(\frac{1}{2\pi}\right)^3\int d\mathbf{q}\,\hat{\lambda}\left(\mathbf{q}\right) < \mathbf{x}|\mathbf{q} > \\ &= \left(\frac{1}{2\pi}\right)^3\int d\mathbf{q}\,\hat{\lambda}\left(\mathbf{q}\right)\exp\left[-2\pi i\mathbf{q}\cdot\mathbf{x}\right] \\ \mathrm{Id} &= \int |\mathbf{q}\rangle\left(\frac{1}{2\pi}\right)^3\langle\mathbf{q}| \\ < \mathbf{p}|\mathbf{q} > &= \left(2\pi\right)^3\delta\left(\mathbf{p}-\mathbf{q}\right) \end{aligned}$$

Then

$$\begin{aligned} \langle\mathbf{k}|\,L\,|\mathbf{h}\rangle &= \int d\mathbf{x}d\mathbf{y}\ < \mathbf{k}|\mathbf{x} >< \mathbf{x}|L|\mathbf{y} >< \mathbf{y}|\mathbf{h} > \\ &= \int d\mathbf{x}\ < \mathbf{k}|\mathbf{x} > \int d\mathbf{y}\,\lambda\left(\mathbf{x}-\mathbf{y}\right) < \mathbf{y}|\mathbf{h} > \\ &= \int d\mathbf{x}\ < \mathbf{k}|\mathbf{x} > \int d\mathbf{y}\,\lambda\left(\mathbf{x}-\mathbf{y}\right) < \mathbf{y}-\mathbf{x}+\mathbf{x}|\mathbf{h} > \\ &= \int d\mathbf{x}\ < \mathbf{k}|\mathbf{x} >< \mathbf{x}|\mathbf{h} > \int \left(-\right)d\mathbf{u}\ < \mathbf{h}|\mathbf{u} >< \mathbf{u}|\lambda > \\ &= - < \mathbf{k}|\mathbf{h} >< \mathbf{h}|\lambda > \\ &= -\left(2\pi\right)^3\delta\left(\mathbf{k}-\mathbf{h}\right)\hat{\lambda}\left(\mathbf{h}\right) \end{aligned}$$

That is L is diagonal in the $|\mathbf{q}>$- basis. Equivalently we can derive $(L^t_{\mathbf{h},\mathbf{k}} = <\mathbf{h}|L^t|\mathbf{k}>)$

$$\begin{aligned} L^t_{\mathbf{h},\mathbf{k}} &= (2\pi)^3 \delta(\mathbf{h}-\mathbf{k}) \hat{\lambda}(-\mathbf{h}) \\ \mathcal{L}_{\mathbf{h},\mathbf{k}} &= \frac{1}{2} (2\pi)^3 \delta(\mathbf{h}-\mathbf{k}) \left(\hat{\lambda}(-\mathbf{h}) - \hat{\lambda}(\mathbf{h})\right) \end{aligned}$$

Next we note that we can suppose that $\lambda(\mathbf{x}) = \lambda(-\mathbf{x})$. This follows from the observation that $P(-\mathbf{x}) = P(\mathbf{x})$ and from the identity $\int d\mathbf{y}\, \rho(\mathbf{y})\, \rho(\mathbf{x}+\mathbf{y}) \equiv \int d\mathbf{y}\, \rho(\mathbf{y})\, \rho(-\mathbf{x}+\mathbf{y})$. Then $\hat{\lambda}(-\mathbf{h}) = -\hat{\lambda}(\mathbf{h})$ and thus

$$\mathcal{L}_{\mathbf{h},\mathbf{k}} = -(2\pi)^3 \delta(\mathbf{h}-\mathbf{k}) \hat{\lambda}(\mathbf{h})$$

Thus $A = -2i\left(\mathcal{L} + \frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)$ is diagonal in the $|\mathbf{q}>$- basis and

$$\begin{aligned} <\mathbf{h}|A|\mathbf{k}> &= A_{\mathbf{h},\mathbf{k}} \\ &= 2i (2\pi)^3 \delta(\mathbf{h}-\mathbf{k}) \left[-\frac{\kappa}{\sqrt{\delta(\mathbf{0})}} + \hat{\lambda}(\mathbf{h})\right] \end{aligned}$$

10.1. Carrying on with the $\mathcal{D}\mu$-integration.

We develop $H[\mu]$ and $\mathcal{H}[\mu]$ along orders of $\delta(\mathbf{0})^{-1}$.

$$
\begin{aligned}
H[\mu] &\equiv H_1[\mu] + \frac{1}{\delta(\mathbf{0})} H_2[\mu] + O\left(\delta(\mathbf{0})^{-2}\right) \\
H_1[\mu] &\equiv H_1^0[\mu] + H_1^1[\mu] \\
H_1^0[\mu] &\equiv E_{\mathbf{h}} E_{\mathbf{k}} E_{-\mathbf{h}-\mathbf{k}}[\rho]\big|_{\rho=-iA^{-1}\mu} \\
&= i \int d\mathbf{u} d\mathbf{v} d\mathbf{z} d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 \ <\mathbf{h}|\mathbf{u}><\mathbf{k}|\mathbf{v}><-\mathbf{h}-\mathbf{k}|\mathbf{z}> \times \\
& A^{-1}_{\mathbf{z},\mathbf{x}_1} \mu(\mathbf{x}_1) A^{-1}_{\mathbf{u},\mathbf{x}_2} \mu(\mathbf{x}_2) A^{-1}_{\mathbf{v},\mathbf{x}_3} \mu(\mathbf{x}_3) \qquad (21) \\
H_1^1[\mu] &\equiv -i \int d\mathbf{u} d\mathbf{v} d\mathbf{z} \ <\mathbf{h}|\mathbf{u}><\mathbf{k}|\mathbf{v}><-\mathbf{h}-\mathbf{k}|\mathbf{z}> \times \\
& \quad \left[\int d\mathbf{y}\, A^{-1}_{\mathbf{z},\mathbf{u}} A^{-1}_{\mathbf{v},\mathbf{y}} \mu(\mathbf{y}) + \int d\mathbf{y}\, A^{-1}_{\mathbf{z},\mathbf{v}} A^{-1}_{\mathbf{u},\mathbf{y}} \mu(\mathbf{y}) + \right. \\
& \quad \left. \int d\mathbf{y}\, A^{-1}_{\mathbf{u},\mathbf{v}} A^{-1}_{\mathbf{z},\mathbf{y}} \mu(\mathbf{y}) \right] \qquad (22) \\
\mathcal{K}^{-1} &= A^{-1} + \frac{1}{\delta(\mathbf{0})} 2i\sqrt{N} A^{-1} M A^{-1} + O\left(\delta(\mathbf{0})^{-2}\right) \\
H_2[\mu] &\equiv H_2^0[\mu] + H_2^1[\mu] \\
\text{where } H_2^0[\mu] &\equiv \text{the } \delta(\mathbf{0})^{-1} \text{ part of } i \int d\mathbf{u} d\mathbf{v} d\mathbf{z} d\mathbf{x}_1 d\mathbf{x}_2 d\mathbf{x}_3 \ <\mathbf{h}|\mathbf{u}><\mathbf{k}|\mathbf{v}><-\mathbf{h}-\mathbf{k}|\mathbf{z}> \times \\
& \mathcal{K}^{-1}_{\mathbf{z},\mathbf{x}_1} \mu(\mathbf{x}_1) \mathcal{K}^{-1}_{\mathbf{u},\mathbf{x}_2} \mu(\mathbf{x}_2) \mathcal{K}^{-1}_{\mathbf{v},\mathbf{x}_3} \mu(\mathbf{x}_3) \\
H_2^1[\mu] &\equiv \text{the } \delta(\mathbf{0})^{-1} \text{ part of } -i \int d\mathbf{u} d\mathbf{v} d\mathbf{z} \ <\mathbf{h}|\mathbf{u}><\mathbf{k}|\mathbf{v}><-\mathbf{h}-\mathbf{k}|\mathbf{z}> \times \\
& \quad \left[\int d\mathbf{y}\, \mathcal{K}^{-1}_{\mathbf{z},\mathbf{u}} \mathcal{K}^{-1}_{\mathbf{v},\mathbf{y}} \mu(\mathbf{y}) + \int d\mathbf{y}\, \mathcal{K}^{-1}_{\mathbf{z},\mathbf{v}} \mathcal{K}^{-1}_{\mathbf{u},\mathbf{y}} \mu(\mathbf{y}) + \right. \\
& \quad \left. \int d\mathbf{z} d\mathbf{y}\, \mathcal{K}^{-1}_{\mathbf{u},\mathbf{v}} \mathcal{K}^{-1}_{\mathbf{z},\mathbf{y}} \mu(\mathbf{y}) \right] \\
\mathcal{H}[\mu] &\equiv 1 + \frac{1}{\delta(\mathbf{0})} \mathcal{H}_1[\mu] \\
\mathcal{H}_1[\mu] &\equiv i\sqrt{N} \mu^t \frac{1}{A} M \frac{1}{A} \mu \\
\alpha &\equiv i\sqrt{N} \left(1 + i \frac{\kappa}{2\sqrt{\delta(\mathbf{0})}} + i\lambda(\mathbf{0}) \frac{\sqrt{N}}{2\delta(\mathbf{0})} \right) \\
\mathcal{H}[\mu] H[\mu] &= \left[\left(1 + \frac{1}{\delta(\mathbf{0})} \mathcal{H}_1[\mu] \right) \left(H_1^0[\mu] + H_1^1[\mu] + \frac{1}{\delta(\mathbf{0})} \left(H_2^0[\mu] + H_2^1[\mu] \right) \right) \right] + O\left(\delta\left(\mathbf{0}^{-2}\right)\right) \\
&= H_1^0[\mu] + H_1^1[\mu] + \frac{1}{\delta(\mathbf{0})} \left[H_2^0[\mu] + H_2^1[\mu] + \mathcal{H}_1[\mu] H_1^0[\mu] + \mathcal{H}_1[\mu] H_1^1[\mu] \right] + O\left(\delta\left(\mathbf{0}^{-2}\right)\right) \qquad (23)
\end{aligned}
$$

Next observe that

1. $H_1^0[\mu]$ is of degree 3 in μ.

2. $H_1^1[\mu]$ is of degree 1 in μ.

3. $H_2^0[\mu]$ is of degree 4 in μ.

4. $H_2^1[\mu]$ is of degree 2 in μ.

5. $\mathcal{H}_1[\mu]\,H_1^0[\mu]$ is of degree 6 in μ.

6. $\mathcal{H}_1[\mu]\,H_1^1[\mu]$ is of degree 4 in μ.

and $\left(\frac{\delta}{\delta\mu}^t A\frac{\delta}{\delta\mu}\right)^p f[\mu]=0$ whenever the degree in μ of f is strictly less than $2p$. Then

$$\exp\left[\frac{1}{2}\frac{\delta}{\delta\mu}^t A\frac{\delta}{\delta\mu}\right] H[\mu]\,\mathcal{H}[\mu]_{\mu=A\alpha} = \left[1+\frac{1}{2}\frac{\delta}{\delta\mu}^t A\frac{\delta}{\delta\mu}+\ldots+\frac{1}{6}\left(\frac{1}{2}\frac{\delta}{\delta\mu}^t A\frac{\delta}{\delta\mu}\right)^3\right] H[\mu]\,\mathcal{H}[\mu]\bigg|_{\mu=A\alpha} + O\left(\delta(\mathbf{0})^{-2}\right)$$

And thus

$$\begin{aligned}
\exp\left[\frac{1}{2}\frac{\delta}{\delta\mu}^t A\frac{\delta}{\delta\mu}\right] H[\mu]\,\mathcal{H}[\mu]\bigg|_{\mu=A\alpha} &= \\
&\left(H_1^0[\mu]+H_1^1[\mu]\right)\Big|_{\mu=A\alpha} + \frac{1}{2}\,\frac{\delta}{\delta\mu}^t A\frac{\delta}{\delta\mu}H_1^0[\mu]\bigg|_{\mu=A\alpha} \\
&+\frac{1}{\delta(\mathbf{0})}\Big\{\left(H_1[\mu]\,\mathcal{H}_1[\mu]+H_2[\mu]\right)_{\mu=A\alpha} + \\
&\frac{1}{2}\frac{\delta}{\delta\mu}^t A\frac{\delta}{\delta\mu}\left(H_1^0[\mu]\,\mathcal{H}_1[\mu]+H_1^1[\mu]\,\mathcal{H}_1[\mu]+H_2^0[\mu]\right)\bigg|_{\mu=A\alpha} + \\
&\frac{1}{8}\left(\frac{\delta}{\delta\mu}^t A\frac{\delta}{\delta\mu}\right)^2\left(H_1^0[\mu]\,\mathcal{H}_1[\mu]+H_1^1[\mu]\,\mathcal{H}_1[\mu]+H_2^0[\mu]\right)_{\mu=A\alpha} + \\
&\frac{1}{48}\left(\frac{\delta}{\delta\mu}^t A\frac{\delta}{\delta\mu}\right)^3\left(H_1^1[\mu]\,\mathcal{H}_1[\mu]\right)\bigg|_{\mu=A\alpha}
\end{aligned}$$

We arrive at the following result

$$I = \int d\kappa \exp\left[\kappa\sqrt{\delta(\mathbf{0})} - \frac{1}{2}\kappa^2\right] \int \mathcal{D}\lambda \exp\left[-\frac{1}{4}\lambda^t (1+\Sigma)\lambda - i\lambda^t \left(Q + i\delta - i\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\delta\right)\right] \times$$

$$\exp\left[iN\left(\lambda^t + \frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)\left(1 + i\frac{\kappa}{2\sqrt{\delta(\mathbf{0})}} + \lambda(\mathbf{0})\frac{\sqrt{N}}{2\delta(\mathbf{0})}\right)^2\right] \sqrt{N}\Big(A^{-1}(\mathbf{h}+\mathbf{k})A^{-1}(\mathbf{h}) +$$

$$A^{-1}(\mathbf{h}+\mathbf{k})A^{-1}(\mathbf{k}) + A^{-1}(\mathbf{h})A^{-1}(\mathbf{k})\Big) \quad (24)$$

where is defined by

$$< \mathbf{p}|A^{-1}|\mathbf{q} > \equiv (2\pi)^3 A^{-1}\delta(\mathbf{p}-\mathbf{q}).$$

Remark that also the common factor $\sqrt{N}$ could have been dropped but we shall still keep it until we have discussed the resulting I

11. Doing the $\mathcal{D}\lambda$-integration

We shall now prepare (25) for the $\mathcal{D}\lambda$-integration. First

$$\begin{aligned}
-\frac{1}{4}\lambda^t(1+\Sigma)\lambda &= -\frac{1}{2}\int d\mathbf{x}\,\lambda(\mathbf{x})^2 \\
&= -\frac{1}{2}\left(\frac{1}{2\pi}\right)^3 \int d\mathbf{p}\,\hat{\lambda}(\mathbf{p})\,\hat{\lambda}(-\mathbf{p}) \\
\frac{1}{2}\int d\mathbf{x}\,\frac{\delta}{\delta\lambda(\mathbf{x})}\frac{\delta}{\delta\lambda(\mathbf{x})} &= \frac{1}{2}\int d\mathbf{x}d\mathbf{p}d\mathbf{q}\,\frac{\delta\hat{\lambda}(\mathbf{p})}{\delta\lambda(\mathbf{x})}\frac{\delta}{\delta\hat{\lambda}(\mathbf{p})}\frac{\delta\hat{\lambda}(\mathbf{q})}{\delta\lambda(\mathbf{x})}\frac{\delta}{\delta\hat{\lambda}(\mathbf{q})} \\
&= 4\pi^3\int d\mathbf{p}\,\frac{\delta}{\delta\hat{\lambda}(\mathbf{p})}\frac{\delta}{\delta\hat{\lambda}(-\mathbf{p})} \\
\mathcal{D}\lambda &\propto \mathcal{D}\hat{\lambda} \\
\lambda^t &\equiv \int d\mathbf{x}\,\lambda(\mathbf{x}) \\
&= \hat{\lambda}^t\delta
\end{aligned}$$

Then (25) can be rewritten

$$I=\int d\kappa\,\exp\left[\kappa\sqrt{\delta(\mathbf{0})}\left(1+\underbrace{\frac{iN}{\delta(\mathbf{0})}\left(1+i\frac{\kappa}{2\sqrt{\delta(\mathbf{0})}}\right)^2}_{\approx 0}\right)-\frac{1}{2}\kappa^2\right]\times$$

$$\int\mathcal{D}\hat{\lambda}\,\exp\left[-\frac{1}{2}\left(\frac{1}{2\pi}\right)^3\int d\mathbf{p}\,\hat{\lambda}(\mathbf{p})\,\hat{\lambda}(-\mathbf{p})-i\hat{\lambda}^t\left(\frac{1}{2\pi}\right)^3\left(\hat{Q}+i-i\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}-N\delta\left(1+i\frac{\kappa}{2\sqrt{\delta(\mathbf{0})}}\right)^2\right)\right]\times$$

$$\left(\frac{1}{\left(\hat{\lambda}(\mathbf{h})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}\frac{1}{\left(\hat{\lambda}(\mathbf{h}+\mathbf{k})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}+\frac{1}{\left(\hat{\lambda}(\mathbf{h}+\mathbf{k})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}\frac{1}{\left(\hat{\lambda}(\mathbf{k})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}+\right.$$

$$\left.\frac{1}{\left(\hat{\lambda}(\mathbf{h})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}\frac{1}{\left(\hat{\lambda}(\mathbf{k})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}\right)$$

Thus according to the formulas for gaussian integration we obtain for I

$$I=\int d\kappa\,\exp\left[\kappa\sqrt{\delta(\mathbf{0})}-\frac{1}{2}\kappa^2-\frac{1}{2}\left(\frac{1}{2\pi}\right)^3\int d\mathbf{p}\,\left(\hat{Q}(\mathbf{p})+i-i\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}-N\delta\left(1+i\frac{\kappa}{2\sqrt{\delta(\mathbf{0})}}\right)^2\right)\right]\times$$

$$\exp\left[\frac{1}{2}(2\pi)^3\int d\mathbf{p}\,\frac{\delta}{\delta\hat{\lambda}(\mathbf{p})}\frac{\delta}{\delta\hat{\lambda}(-\mathbf{p})}\right]\times\left(\frac{1}{\left(\hat{\lambda}(\mathbf{h})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}\frac{1}{\left(\hat{\lambda}(\mathbf{h}+\mathbf{k})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}+\right.$$

$$\left.\frac{1}{\left(\hat{\lambda}(\mathbf{h}+\mathbf{k})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}\frac{1}{\left(\hat{\lambda}(\mathbf{k})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}+\frac{1}{\left(\hat{\lambda}(\mathbf{h})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}\frac{1}{\left(\hat{\lambda}(\mathbf{k})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}\right)$$

$$\text{at }\hat{\lambda}=-i\frac{(2\pi)^3}{(2\pi)^3}\left(\hat{Q}+i-i\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}-N\delta\left(1+i\frac{\kappa}{2\sqrt{\delta(\mathbf{0})}}\right)^2\right)$$

$$\hat{Q}(\mathbf{p})=R_{\mathbf{p}}^2-1$$

Next remark that

$$\begin{aligned}\text{Integration over reciprocal space }\int d\mathbf{p}&=\int d\mathbf{p}\,e^{2i\pi\mathbf{p}\cdot\mathbf{0}}\\&=(2\pi)^3\,\delta(\mathbf{0})\end{aligned}$$

Every differentiation $\frac{\delta}{\delta\hat{\lambda}(\mathbf{p})}$ acting on e.g. $\frac{1}{\left(\hat{\lambda}(\mathbf{h})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}$ gives us back again a multiple of a power of $\frac{1}{\left(\hat{\lambda}(\mathbf{h})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}$. So we see that $\frac{\delta}{\delta\hat{\lambda}(\mathbf{p})}\frac{1}{\left(\hat{\lambda}(\mathbf{h})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}$ at $\hat{\lambda}=-i\left(\hat{Q}+i-i\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}-N\delta\left(1+i\frac{\kappa}{2\sqrt{\delta(\mathbf{0})}}\right)^2\right)$

becomes

$$\frac{\delta}{\delta\hat{\lambda}(\mathbf{p})}\frac{1}{\hat{\lambda}(\mathbf{h})}\text{ at }\hat{\lambda}=-i\left(\hat{Q}+i-N\delta\left(1+i\frac{\kappa}{2\sqrt{\delta(\mathbf{0})}}\right)^2\right)$$

Also because $\delta(\mathbf{h})=0$ $(\mathbf{h}\neq\mathbf{0})$ we see that $\frac{\delta}{\delta\hat{\lambda}(\mathbf{p})}\frac{1}{\left(\hat{\lambda}(\mathbf{h})+\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}\right)}$ at $\hat{\lambda}=-i\left(\hat{Q}+i-i\frac{\kappa}{\sqrt{\delta(\mathbf{0})}}-N\delta\left(1+i\frac{\kappa}{2\sqrt{\delta(\mathbf{0})}}\right)^2\right)$ is nothing else but

$$\frac{\delta}{\delta\hat{\lambda}(\mathbf{p})}\frac{1}{\hat{\lambda}(\mathbf{h})}\text{ at }\hat{\lambda}=-i\left(\hat{Q}+i\right)$$

Since κ has disappeard in this expression we can throw the κ-integral away and we obtain

$$I=Cte\exp\left[4\pi^3\int d\mathbf{p}\,\frac{\delta}{\delta\hat{\lambda}(\mathbf{p})}\frac{\delta}{\delta\hat{\lambda}(-\mathbf{p})}\right]\times\sqrt{N}\left(\frac{1}{\hat{\lambda}(\mathbf{h})}\frac{1}{\hat{\lambda}(\mathbf{h}+\mathbf{k})}+\frac{1}{\hat{\lambda}(\mathbf{h}+\mathbf{k})}\frac{1}{\hat{\lambda}(\mathbf{k})}+\frac{1}{\hat{\lambda}(\mathbf{h})}\frac{1}{\hat{\lambda}(\mathbf{k})}\right)\text{ at }\hat{\lambda}=-i\left(\hat{Q}+i\right)\tag{25}$$

Let's write the first order approximation of this expression (we throw away $\frac{1}{(-i)^2}$)

$$I_{\text{first order}}=\sqrt{N}\left[\frac{1}{\left(\hat{Q}_{\mathbf{h}}+i\right)\left(\hat{Q}_{\mathbf{h}+\mathbf{k}}+i\right)}+\frac{1}{\left(\hat{Q}_{\mathbf{k}}+i\right)\left(\hat{Q}_{\mathbf{h}+\mathbf{k}}+i\right)}+\frac{1}{\left(\hat{Q}_{\mathbf{h}}+i\right)\left(\hat{Q}_{\mathbf{k}}+i\right)}\right]\tag{26}$$

(since $\sqrt{N}$ is an overall constant we can safely drop it). We are not interested in the renormalizing constant since we don't know the probability distribution. We see that for very high $\hat{R}_{\mathbf{h}}\approx\hat{R}_{\mathbf{k}}\approx\hat{R}_{\mathbf{h}+\mathbf{k}}$ the complex number $I_{\text{first order}}$ becomes almost positive which makes sense.

The next order for I is obtained after functional derivation $4\pi^3\int d\mathbf{p}\,\frac{\delta}{\delta\hat{\lambda}(\mathbf{p})}\frac{\delta}{\delta\hat{\lambda}(-\mathbf{p})}$ applied to $\frac{1}{\hat{\lambda}(\mathbf{h})}\frac{1}{\hat{\lambda}(\mathbf{h}+\mathbf{k})}+\frac{1}{\hat{\lambda}(\mathbf{h}+\mathbf{k})}\frac{1}{\hat{\lambda}(\mathbf{k})}+\frac{1}{\hat{\lambda}(\mathbf{h})}\frac{1}{\hat{\lambda}(\mathbf{k})}$. For instance

$$4\pi^3\int d\mathbf{p}\,\frac{\delta}{\delta\hat{\lambda}(\mathbf{p})}\frac{\delta}{\delta\hat{\lambda}(-\mathbf{p})}\frac{1}{\hat{\lambda}(\mathbf{h})}\frac{1}{\hat{\lambda}(\mathbf{k})}\bigg|_{\hat{\lambda}=\hat{Q}+i}=4\pi^3\left(\frac{6}{\left(\hat{Q}_{\mathbf{h}}+i\right)^3\left(\hat{Q}_{\mathbf{k}}+i\right)}+\frac{6}{\left(\hat{Q}_{\mathbf{h}}+i\right)\left(\hat{Q}_{\mathbf{k}}+i\right)^3}+\frac{2}{\left(\hat{Q}_{\mathbf{h}}+i\right)^2\left(\hat{Q}_{\mathbf{k}}+i\right)^2}\right.$$

References

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